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Letters to the Editor

Effect of lattice vibrations on the exchange-interaction in ferro—and anti-ferro-magnetic crystals.

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Heisenberg (1928) for the first time gave the most successful interpretation of the origin of the apparently enormous but mysterious Weiss molecular field in a ferromagnetic in terms of exchange interaction between spins of the electrons on neighbouring atoms in a crystal lattice. According to this localized-spin model for a magnetic solid, it is well known, that the Hamiltonian of the spin system is given by $H = -2J \Sigma_{n.i} S_i S_j \cdots(1)$, besides the zeeman energy of the spins, where S_i is the spin vector of the ith atom, measured in multiples of $\frac{\hbar}{2}$. The term in equation (1) is the exchange energy and contains the familiar exchange integral J and the summation extends only over the neighbouring atoms. The equation (1) in the more general case takes the form $-2\Sigma_{j>i} J_{ij} S_i S_j$ and the sum runs over all pairs of atoms in the crystal. The magnitude of the exchange coupling constant J, between adjacent atoms, is positive for ferromagnetics and negative for antiferromagnetics. The magnitude of J, is dependent on the ratio of the radius of the atom (half the internuclear distant in the crystal) to the effective radius of the incomplete 3d or 4f shell of the atoms. The outstanding feature of the Heisenberg theory of ferromagnetism lies in showing the dependence of the Curie temperature as also of the Weiss molecular field constant on the strength of J.

Bethe (1933) showed that the exchange integral J is positive in the case of Fe, Co, and Ni (incomplete 3d shell) and Gd and Dy (incomplete 4f shell) only in the special circumstances when the ratio of the radius the R of the atom to the radius γ of the imcomplete 3d or 4f shell is within a certain limited range and had shown the variation of J for the ferromagnetic element with R/r. Neél (1936, 1946) calculated the ratio $U = \theta_C / C_A Z$ known as reduced molecular field coeficient where Z is the number of nearest neighbours of an atom C_A the usual Curie constant for a gm. atom. This reduced molecular field coefficient is also dependent on J. A more generalised curve showing the variation of U (positive for ferromagnetics and negative for antiferromagnetics with $(d\text{-}2r)$ has been drawn by Neél

(1940) and reported by Stoner (1946-47) where d is interatomic distance and r is the effective radius of the d shell.

Born (1942) in his theory of the intensity of diffuse spots due to scattered X-radiation, on the basis of lattice dynamics, has introduced the concept of a dynamic lattice constant

$$l = \frac{\hbar}{(mk\theta_D)^{1/2}} = \frac{6.96\times10^{-8}}{(\mu\theta_D)^{1/2}} \text{ cm.}$$

as the root mean square amplitude of a linear oscillator of frequency $W_0 = k\theta_D/\hbar$, where m = mass of the atom, k = Boltzmann constant μ = atomic mass in atomic units and θ_D = Debye temperature. As such $ml^2\omega_0^2 = \hbar\omega_0 = k\theta_D$ (energy of lattice vibrations)

In this note some aspects of correlations due to the influence of Bohr's dynamic lattice constant in the variation of the reduced moleeular field coefficient of Neél with $(d\text{-}2r)$ have been shown. Figure 1 contains two

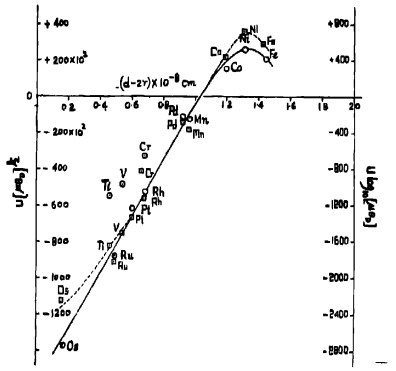

Figure 1.

(a) Thick lined curve showing the variation of $U(\mu\theta_D)^{1/2}$ vs. $(d-2r)$.

(b) Dotted curve showing the variation of $U \log(\mu\theta_D)$ vs. $(d\text{-}2r)$

curves, one showing the variation of U $(\mu\theta_D)^{1/2}$ (proportional to U/l) vs.$(d\text{-}2r)$ $\times$ 10^{-8} cm. and the other showing the variation of U log $(\mu\theta_D)$ vs.$(d\text{-}2r)$ $\times$ 10^{-8} cm. Figure 2 shows two curves, showing the variations as noted in the captions below.

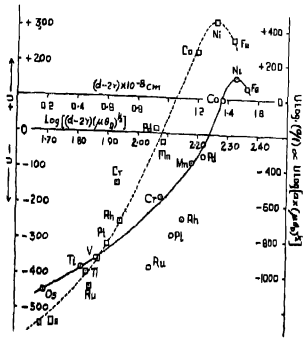

Figure 2. *(a)* Thick lined curve showing the variation of U vs $\log (d-2r)(\mu\theta_D)^{\frac{1}{2}}$

(b) Dotted curve showing the variation of U log a/l or U log $a(\mu\theta_D)^{\frac{1}{2}}$ vs. $(d-2r)$ where 'a' is the lattice constant.

Figure 3 shows the variation of U vs. l^{-1}, *i.e*, U vs. $(\mu\theta_D)^{1/2}$. These curves bear significance and it is really interesting to find that the nature of the curves in figure 1 and 2 are very similar to that of U *vs.* $(d\text{-}2r)$ curve of Neél. The curve of figure 3 clearly indicates a sharp rise in the value of U for Fe, Co, Ni within a certain limited range of $(\mu\theta_D)^{1/2}$ which also means within a limited range of the dynamic lattice constant. It is very significant that l^{-1} which is proportional to $(\mu\theta_D)^{1/2}$ or some function of $(\mu\theta_D)^{1/2}$ like log $(\mu\theta_D)^{1/2}$ is linked up with the reduced molecular field cofficient of Neel in such a way as to make it vary with $(d\text{-}2r)$ much in the same manner as the curve of Neél. Various types of interaction processes can occur involving phonons and magnons. Lattice vibrations, depending

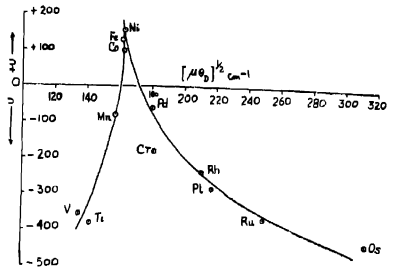

Figure 3. Showing variation of U vs. $(\mu\theta_D)^{1/2}$

on temperature, destroy perfect lattice periodicity in a crystal and produce time-dependent imperfection in the lattice. Spin waves couple first to one another and then to the lattice by the process or magnon-phonon coupling. Further Sinha & Upadhyaya (1962) and Upadhyaya & Sinha (1963) have shown the dispersion relation of magnon energy to be given by $\hbar\omega_\lambda = 2JSK_\lambda^2a^2$ for a ferromagnetic and $2JSK_\lambda a$ (approximately) for an antiferromagnetic crystal, where K_λ = reduced wave vector and a = lattice constant. Variation of U log as a function of $(d\text{-}2r)$ has been shown in one of the curves of figure 2. The values of U and $(d\text{-}2r)$ have been taken from Neél's work (1940) and those of θ_D from the table in Gray's book (1963).

These aspects of correlations reflect the effect of lattice vibrations on the exchange interaction constant J and provide phenomenologically an insight into the manifestation of the phonon-modified exchange which plays an important role in the mechanism of the magnon-phonon or spin-phonon interactions worked out by Sinha *et al* (1963) and Bakre, *et al* (1667). These aspects of correlations also suggest the fundamental nature of Born's dynamic lattice constant. It is apparent that there will be also a spin-phonon interaction effect on the well known Debye (1914) Waller (1923, 1925) factor modifying the intensity of X-ray diffraction maxima. Further work on these aspects in progress.

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